9-AMA

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 186 °C

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 3.39e-01

Nearest Neighbors from the Training Set

Image not found
9-Aminoacridine
Measured: 241
Predicted: 172

Image not found
4-Aminoacridine
Measured: 108
Predicted: 153

Image not found
Ellipticine
Measured: 313
Predicted: 195

Image not found
Phenazine
Measured: 177
Predicted: 127